201-16560B

# IUCLID

# Data Set

| | | |
|---|---|---|
| **Existing Chemical** | : | ID: 74-86-2 |
| **CAS No.** | : | 74-86-2 |
| **EINECS Name** | : | acetylene |
| **EC No.** | : | 200-816-9 |
| **TSCA Name** | : | Ethyne |
| **Molecular Formula** | : | C2H2 |
| | | |
| **Producer related part** | | |
| **Company** | : | PCA Services, Inc |
| **Creation date** | : | 15.08.2003<br>For American Chemistry Council |
| **Substance related part** | | |
| **Company** | : | PCA Services, Inc |
| **Creation date** | : | 15.08.2003<br>For American Chemistry Council |
| **Status** | : | |
| **Memo** | : | |
| | | |
| **Printing date** | : | 23.02.2007 |
| **Revision date** | : | 23.02.2007 |
| **Date of last update** | : | 23.02.2007 |
| | | |
| **Number of pages** | : | 36 |
| | | |
| **Chapter (profile)** | : | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile)** | : | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile)** | : | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

## 1.0.1 APPLICANT AND COMPANY INFORMATION

| | | |
|---|---|---|
| **Type** | : | Sponsor: |
| **Name** | : | American Chemistry Council<br>Acetylene Panel |
| **Contact person** | : | Nancy Sandrof |
| **Date** | : | |
| **Street** | : | 1300 Wilson Boulevard |
| **Town** | : | 22209 Arlington, VA |
| **Country** | : | United States |
| **Phone** | : | 1-703-741-5605 |
| **Telefax** | : | 1-703-741-6091 |
| **Telex** | : | |
| **Cedex** | : | |
| **Email** | : | |
| **Homepage** | : | |

19.11.2004

| | | |
|---|---|---|
| **Type** | : | |
| **Name** | : | Acetylene Panel Members: Air Liquide America Company; BASF Corporation; Chevron Phillips Chemical Company; The Dow Chemical Company; DuPont; Equistar Chemicals LP; Praxair, Inc.; Rohm and Haas Company; and Shell Chemicals Limited. |
| **Contact person** | : | Nancy Sandrof (see above) |
| **Date** | : | |
| **Street** | : | |
| **Town** | : | |
| **Country** | : | |
| **Phone** | : | |
| **Telefax** | : | |
| **Telex** | : | |
| **Cedex** | : | |
| **Email** | : | |
| **Homepage** | : | |

## 1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

## 1.0.3 IDENTITY OF RECIPIENTS

## 1.0.4 DETAILS ON CATEGORY/TEMPLATE

## 1.1.0 SUBSTANCE IDENTIFICATION

| | | |
|---|---|---|
| **IUPAC Name** | : | ethyne |
| **Smiles Code** | : | C#C |
| **Molecular formula** | : | C2H2 |
| **Molecular weight** | : | 26.04 |
| **Petrol class** | : | |

**Reliability** : (1) valid without restriction
15.08.2003

### 1.1.1 GENERAL SUBSTANCE INFORMATION

**Purity type** : typical for marketed substance
**Substance type** : organic
**Physical status** : gaseous
**Purity** : >=
**Colour** : colorless, clear
**Odour** : faint ether or garlic like odor

15.08.2003 (24)

### 1.1.2 SPECTRA

### 1.2 SYNONYMS AND TRADENAMES

**ethyne**

**Reliability** : (1) valid without restriction
03.01.2007

### 1.3 IMPURITIES

**Purity** :
**CAS-No** : 7803-51-2
**EC-No** : 232-260-8
**EINECS-Name** : phosphine
**Molecular formula** : H3P
**Value** :

**Remark** : Phosphine is an impurity, when acetylene is produced from calcium carbide. This is a minor process for the manufacture of acetylene.

04.01.2007

**Purity** :
**CAS-No** : 7783-06-4
**EC-No** : 231-977-3
**EINECS-Name** : hydrogen sulphide
**Molecular formula** : H2S
**Value** :

04.01.2007

**Purity** :
**CAS-No** : 7784-42-1
**EC-No** : 232-066-3
**EINECS-Name** : arsine
**Molecular formula** : AsH3
**Value** :

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**Purity** :
**CAS-No** : 7664-41-7
**EC-No** : 231-635-3
**EINECS-Name** : ammonia, anhydrous
**Molecular formula** : NH3
**Value** :

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## 1.4 ADDITIVES

## 1.5 TOTAL QUANTITY

## 1.6.1 LABELLING

## 1.6.2 CLASSIFICATION

## 1.6.3 PACKAGING

## 1.7 USE PATTERN

**Type of use** : industrial
**Category** : Basic industry: basic chemicals

03.01.2007 (25)

## 1.7.1 DETAILED USE PATTERN

**Industry category** : 2 Chemical industry: basic chemicals
**Use category** :
**Extra details on use category** : No extra details necessary
No extra details necessary
**Emission scenario document** : not available
**Product type/subgroup** :
**Tonnage for Application** :
**Year** :
**Fraction of tonnage for application** :
**Fraction of chemical in formulation** :
**Production** : :
**Formulation** : :
**Processing** : :
**Private use** :
**Recovery** :

**Remark** : Used as a chemical intermediate in the manufacture of other chemicals (ca. 80% of manufacture) and in acetylene welding (ca. 20% of manufacture).
**Reliability** : (1) valid without restriction
04.01.2007 (20)

### 1.7.2 METHODS OF MANUFACTURE

**Origin of substance** : Synthesis
**Type** : Production

**Result** : The major producers in the U.S. manufacture acetylene by either the partial oxidation of natural gas or as a co-product from the steam cracking of ethylene. Acetylene can be produced also by the reaction of calcium carbide with water, but this is a minor means of production.
**Reliability** : (1) valid without restriction
04.01.2007 (19) (20)

### 1.8 REGULATORY MEASURES

### 1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

### 1.8.2 ACCEPTABLE RESIDUES LEVELS

### 1.8.3 WATER POLLUTION

### 1.8.4 MAJOR ACCIDENT HAZARDS

### 1.8.5 AIR POLLUTION

### 1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

### 1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

### 1.9.2 COMPONENTS

### 1.10 SOURCE OF EXPOSURE

**Source of exposure** : Human: exposure of the operator by intended use
**Exposure to the** : Substance

**Remark** : Use of acetylene as an industrial intermediate (which amounts to 80% of production) is carried out in enclosed systems, because any meaningful escape of this gas presents a serious explosion hazard. Therefore any human exposure by inhalation (the only meaningful route) would be insignificant.
**Reliability** : (2) valid with restrictions
04.01.2007 (25)

**Source of exposure** : Human: exposure of the consumer/bystander
**Exposure to the** : Substance

**Remark** : Acetylene is not expected or known to be present in significant concentrations in consumer products. Therefore consumer exposure is not expected to be significant.
**Reliability** : (2) valid with restrictions
04.01.2007 (25)

**Source of exposure** : Human: exposure through intended use
**Exposure to the** : Substance

**Remark** : About 20% of production is used in welding. The most likely scenario for human exposure to acetylene (inhalation being the only likely route) is during its use in small welding shops where welding is not automated and/or may not include engineering controls. It is possible that at the start of a welding operation, when the welding torch is ignited, a very small amount of acetylene may escape without combustion in the split second when the valve to the acetylene tank is opened and before ignition. It is inconceivable, however, that the amount liberated in this extremely short interval would be sufficient to contribute significantly to an appreciable room concentration of acetylene. Once ignition takes place, the acetylene is completely consumed by combustion (the temperature of the welding torch is > 3300 degrees C). If that were not the case, a serious explosion hazard could develop through gradual concentration build-up. In fact, acetylene welding has been conducted daily without incident (except in very rare cases) in many locations for decades. This well established, de facto record of safety in acetylene welding supports the absence of acetylene air concentration buildup during welding operations.
**Reliability** : (2) valid with restrictions
04.01.2007 (25)

**Source of exposure** : Human: exposure by production
**Exposure to the** : Substance

**Remark** : Acetylene is and must be manufactured in a closed system, because any meaningful escape of even minor amounts of this gas presents a serious fire or explosion hazard. Therefore any human exposure by inhalation (the only meaningful route) would be insignificant.
**Reliability** : (2) valid with restrictions
04.01.2007 (25)

## 1.11 ADDITIONAL REMARKS

## 1.12 LAST LITERATURE SEARCH

## 1.13 REVIEWS

### 2.1 MELTING POINT

| | | |
|---|---|---|
| **Value** | : | = -80.8 °C |
| **Sublimation** | : | |
| **Method** | : | other |
| **Year** | : | |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Reliability** | : | (2) valid with restrictions<br>Peer reviewed data that came from a reliable reference textbook. |
| **Flag** | : | Critical study for SIDS endpoint |

15.08.2003 (21)

### 2.2 BOILING POINT

| | | |
|---|---|---|
| **Value** | : | = -84 °C at 1016 hPa |
| **Decomposition** | : | |
| **Method** | : | other |
| **Year** | : | |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Sublimes at boiling point. Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983. 154. |
| **Reliability** | : | (2) valid with restrictions<br>Peer reviewed data that came from a reliable reference textbook. |
| **Flag** | : | Critical study for SIDS endpoint |

15.08.2003 (21)

### 2.3 DENSITY

| | | |
|---|---|---|
| **Type** | : | relative density |
| **Value** | : | = .6208 at -82 °C |
| **Method** | : | other |
| **Year** | : | |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Reliability** | : | (2) valid with restrictions<br>Peer reviewed data that came from a reliable reference textbook. |

15.08.2003 (21)

### 2.3.1 GRANULOMETRY

### 2.4 VAPOUR PRESSURE

| | | |
|---|---|---|
| **Value** | : | = 6969.2 hPa at 25 °C |
| **Decomposition** | : | |
| **Method** | : | other (calculated) |
| **Year** | : | |
| **GLP** | : | no |

| | | |
|---|---|---|
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Vapor pressure calculated from experimentally derived coefficients. |
| **Result** | : | Vapor pressure = 40 ATM @ 16.8 DEG C.<br>Sax, N.I. Dangerous Properties of Industrial Materials. 6th ed. New York, NY: Van Nostrand Reinhold, 1984. 107. |
| **Reliability** | : | (2) valid with restrictions<br>Peer reviewed data that came from a reliable reference textbook. |
| **Flag** | : | Critical study for SIDS endpoint |

15.08.2003 (3)

### 2.5 PARTITION COEFFICIENT

| | | |
|---|---|---|
| **Partition coefficient** | : | octanol-water |
| **Log pow** | : | = .37 at 20 °C |
| **pH value** | : | = 7 |
| **Method** | : | other (calculated) |
| **Year** | : | 1995 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Reliability** | : | (2) valid with restrictions<br>Data calculated by a reliable source using a recognized, documented estimation method. |
| **Flag** | : | Critical study for SIDS endpoint |

03.01.2007 (15)

### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

| | | |
|---|---|---|
| **Solubility in** | : | Water |
| **Value** | : | = 1230 mg/l at 20 °C |
| **pH value** | : | = 7 |
| **concentration** | : | at °C |
| **Temperature effects** | : | |
| **Examine different pol.** | : | |
| **pKa** | : | at 25 °C |
| **Description** | : | |
| **Stable** | : | |
| **Result** | : | 1230 mg/l at 20 °C and 1013 hPa |
| **Reliability** | : | (2) valid with restrictions<br>Data came from a reliable reference textbook. |
| **Flag** | : | Critical study for SIDS endpoint |

04.01.2007 (14)

| | | |
|---|---|---|
| **Solubility in** | : | Water |
| **Value** | : | = 1200 mg/l at 25 °C |
| **pH value** | : | = 7 |
| **concentration** | : | at °C |
| **Temperature effects** | : | |
| **Examine different pol.** | : | |
| **pKa** | : | at 25 °C |
| **Description** | : | |
| **Stable** | : | |
| **Reliability** | : | (2) valid with restrictions<br>Data are from a secondary source. The primary source is a reliable reference textbook that was not consulted. |

04.01.2007 (26)

### 2.6.2 SURFACE TENSION

### 2.7 FLASH POINT

### 2.8 AUTO FLAMMABILITY

### 2.9 FLAMMABILITY

| | | |
|---|---|---|
| **Result** | **:** | extremely flammable |
| **Method** | **:** | other |
| **Year** | **:** | |
| **GLP** | **:** | no |
| **Test substance** | **:** | as prescribed by 1.1 - 1.4 |
| **Result** | **:** | Flammable Limits: Upper: 100% by vol.; Lower 2.5% by vol. |
| **Reliability** | **:** | (2) valid with restrictions |

15.08.2003 (12)

### 2.10 EXPLOSIVE PROPERTIES

### 2.11 OXIDIZING PROPERTIES

### 2.12 DISSOCIATION CONSTANT

### 2.13 VISCOSITY

### 2.14 ADDITIONAL REMARKS

### 3.1.1 PHOTODEGRADATION

| | | |
|---|---|---|
| **Type** | : | air |
| **Light source** | : | Sun light |
| **Light spectrum** | : | nm |
| **Relative intensity** | : | based on intensity of sunlight |
| **INDIRECT PHOTOLYSIS** | | |
| **Sensitizer** | : | OH |
| **Conc. of sensitizer** | : | |
| **Rate constant** | : | = .000000000000815 $cm^3$/(molecule*sec) |
| **Degradation** | : | = 50 % after 13.1 day(s) |
| **Deg. product** | : | |
| **Method** | : | other (calculated) |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Measured inputs to the program were melting point (-80.8 degrees C), boiling point (-84 degrees C), vapor pressure (5240 mm Hg) and water solubility (1,200 mg/l). |
| **Reliability** | : | (2) valid with restrictions<br>Data were estimated using a model. |
| **Flag** | : | Critical study for SIDS endpoint |

04.01.2007 (2) (6)

### 3.1.2 STABILITY IN WATER

| | | |
|---|---|---|
| **Deg. product** | : | |
| **Method** | : | other (calculated) |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Measured inputs to the program were melting point (-80.8 degrees C), boiling point (-84 degrees C), vapor pressure (5240 mm Hg) and water solubility (1,200 mg/l). |
| **Result** | : | EPIWIN Hydrowin cannot calculate hydrolysis rate constant for molecular structures of the acetylene type. Hydrolysis of acetylene in water is likely to be an unimportant pathway, because acetylene does not possess a functional group known to be susceptible to hydrolysis at neutral ambient conditions. Also, despite acetylene's measurable solubility in water, acetylene has a pronounced tendency to quickly volatilize from water to the atmosphere, based on its high vapor pressure and existence as a gas at ambient temperature. |
| **Reliability** | : | (3) invalid<br>EPIWIN Hydrowin Model cannot estimate hydrolysis of acetylene. |

04.01.2007 (11)

### 3.1.3 STABILITY IN SOIL

### 3.2.1 MONITORING DATA

### 3.2.2 FIELD STUDIES

### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

| | | |
|---|---|---|
| **Type** | : | fugacity model level III |
| **Media** | : | other: air, water, soil, sediment |
| **Air** | : | 99.9 % (Fugacity Model Level I) |
| **Water** | : | .104 % (Fugacity Model Level I) |
| **Soil** | : | % (Fugacity Model Level I) |
| **Biota** | : | .0002 % (Fugacity Model Level II/III) |
| **Soil** | : | .0101 % (Fugacity Model Level II/III) |
| **Method** | : | other |
| **Year** | : | 2003 |
| **Result** | : | Estimated half-lives in various media are: air = 298 hours, water = 360 hours, soil = 360 hours and sediment = 1440 hours. The soil/sediment constant Koc = 14.3, as estimated by the EPIWIN PcKoc Program (v1.66). The Henry's Law Constant calculated by EPIWIN Henry (v3.10) = 2.40 E-002 atm-m3/mole. |
| **Test condition** | : | Measured inputs to the program were melting point (-80.8 degrees C), boiling point (-84 degrees C), vapor pressure (5240 mm Hg) and water solubility (1,200 mg/l). The emission rate values of 1000 kg/hr to air, and 0 kg/hr to water, sediment and soil were inputted. |
| **Reliability** | : | (2) valid with restrictions<br>Data were calculated using a well-recognized computer estimation program. |
| **Flag** | : | Critical study for SIDS endpoint |

03.01.2007 (10)

### 3.3.2 DISTRIBUTION

### 3.4 MODE OF DEGRADATION IN ACTUAL USE

### 3.5 BIODEGRADATION

| | | |
|---|---|---|
| **Deg. product** | : | |
| **Method** | : | other: calculated |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Measured inputs to the program were melting point (-80.8 degrees C), boiling point (-84 degrees C), vapor pressure (5240 mm Hg) and water solubility (1,200 mg/l). |
| **Result** | : | EPIWIN BIOWIN (v4.00) predicts ready biodegradability using both nonlinear and linear methods |
| **Reliability** | : | (2) valid with restrictions<br>Data were obtained by modeling. |
| **Flag** | : | Critical study for SIDS endpoint |

28.12.2006 (8)

### 3.6 BOD5, COD OR BOD5/COD RATIO

## 3.7 BIOACCUMULATION

| | | |
|---|---|---|
| **Species** | : | other |
| **Exposure period** | : | at 25 °C |
| **Concentration** | : | |
| **BCF** | : | = 3.16 |
| **Elimination** | : | |
| **Method** | : | other: calculated |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Measured inputs to the program were melting point (-80.8 degrees C), boiling point (-84 degrees C), vapor pressure (5240 mm Hg) and water solubility (1,200 mg/l). |
| **Reliability** | : | (2) valid with restrictions<br>Data estimated using a computer program. |

15.08.2003 (7)

## 3.8 ADDITIONAL REMARKS

## 4.1 ACUTE/PROLONGED TOXICITY TO FISH

| | | |
|---|---|---|
| **Type** | : | other: estimation |
| **Species** | : | other |
| **Exposure period** | : | 96 hour(s) |
| **Unit** | : | mg/l |
| **LC50** | : | = 496.148 calculated |
| **Limit test** | : | |
| **Analytical monitoring** | : | no |
| **Method** | : | other: calculated |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Measured inputs to the program were melting point (-80.8 degrees C), boiling point (-84 degrees C), vapor pressure (5240 mm Hg) and water solubility (1,200 mg/l).<br><br>This is a supporting study for the SIDS endpoint. |
| **Reliability** | : | (2) valid with restrictions<br>Data were calculated using a computer program. |

28.12.2006 (9)

| | | |
|---|---|---|
| **Type** | : | other: no data |
| **Species** | : | Lepomis sp. |
| **Exposure period** | : | 1 hour(s) |
| **Unit** | : | |
| **Method** | : | other |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Exposure of sunfish to 1000 ppm acetylene (at 18 degrees C) did not result in death. No other information was provided.<br><br>This is a supporting study for the SIDS endpoint. |
| **Source** | : | The primary source of the data was not cited in the OHM/TADS data file. |
| **Reliability** | : | (4) not assignable<br>There are not enough details to assign a reliability rating. |

04.01.2007 (22)

| | | |
|---|---|---|
| **Type** | : | other: no data |
| **Species** | : | other: minnow |
| **Exposure period** | : | 1 hour(s) |
| **Unit** | : | |
| **Method** | : | other |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Exposure of minnows (no species indicated) to 17 ppm acetylene in well-oxygenated water had no effect.<br><br>This is a supporting study for the SIDS endpoint. |
| **Source** | : | The primary source of the data was not cited in the OHM/TADS data file. |
| **Reliability** | : | (4) not assignable<br>There are not enough details to assign a reliability rating. |

04.01.2007 (22)

| | | |
|---|---|---|
| **Type** | : | other: no data |
| **Species** | : | other: trout fingerlings |
| **Exposure period** | : | 33 hour(s) |
| **Unit** | : | mg/l |
| **Method** | : | other |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Remark** : Exposure of trout fingerlings to 200 ppm acetylene at 10-14 degrees C resulted in death to an unlisted number of fish.

This is a supporting study for the SIDS endpoint.

**Source** : The primary source of the data was not cited in the OHM/TADS data file.
**Reliability** : (4) not assignable
There are not enough details to assign a reliability rating.

04.01.2007 (22)

| | | |
|---|---|---|
| **Type** | : | other: no data |
| **Species** | : | Cyprinus auratus |
| **Exposure period** | : | |
| **Unit** | : | mg/l |
| **Method** | : | other |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Remark** : Exposure of goldfish to 400 ppm acetylene for 24 to 48 hours resulted in death to an unlisted number of fish.

This is a supporting study for the SIDS endpoint.

**Source** : The primary source of the data was not cited in the OHM/TADS data file.
**Reliability** : (4) not assignable
There are not enough details to assign a reliability rating.

04.01.2007 (22)

| | | |
|---|---|---|
| **Type** | : | other |
| **Species** | : | other:fingerling chinook salmon |
| **Exposure period** | : | 72 hour(s) |
| **Unit** | : | |
| **Method** | : | other |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Remark** : The "critical level" at 72 hours for fingerling Chinook salmon in brackish water was 3500 ppm.

This is a supporting study for the SIDS endpoint.

**Source** : The primary source of the data was not cited in the OHM/TADS data file.
**Reliability** : (4) not assignable
There are not enough details to assign a reliability rating.

04.01.2007 (22)

| | | |
|---|---|---|
| **Type** | : | other: no data |
| **Species** | : | other: young rainbow trout |
| **Exposure period** | : | 72 hour(s) |
| **Unit** | : | |
| **Method** | : | other |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

| | | |
|---|---|---|
| **Remark** | : | The "critical level" at 72 hours for young rainbow trout in fresh water was 3000 - 5000 ppm.<br><br>This is a supporting study for the SIDS endpoint. |
| **Source** | : | The primary source of the data was not cited in the OHM/TADS data file. |
| **Reliability** | : | (4) not assignable<br>There are not enough details to assign a reliability rating. |

04.01.2007 (22)

## 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

| | | |
|---|---|---|
| **Type** | : | other: calculated |
| **Species** | : | Daphnia magna (Crustacea) |
| **Exposure period** | : | 48 hour(s) |
| **Unit** | : | mg/l |
| **EC50** | : | = 479.304 calculated |
| **Analytical monitoring** | : | no |
| **Method** | : | other: calculated |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Measured inputs to the program were melting point (-80.8 degrees C), boiling point (-84 degrees C), vapor pressure (5240 mm Hg) and water solubility (1,200 mg/l). |
| **Reliability** | : | (2) valid with restrictions<br>Data were calculated using a computer program. |
| **Flag** | : | Critical study for SIDS endpoint |

28.12.2006 (9)

## 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

| | | |
|---|---|---|
| **Species** | : | other algae: green algae |
| **Endpoint** | : | growth rate |
| **Exposure period** | : | 96 hour(s) |
| **Unit** | : | mg/l |
| **EC50** | : | = 274.86 calculated |
| **Limit test** | : | |
| **Analytical monitoring** | : | no |
| **Method** | : | other: calculated |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Measured inputs to the program were melting point (-80.8 degrees C), boiling point (-84 degrees C), vapor pressure (5240 mm Hg) and water solubility (1,200 mg/l). |
| **Reliability** | : | (2) valid with restrictions<br>Data were estimated by a computer program. |
| **Flag** | : | Critical study for SIDS endpoint |

28.12.2006 (9)

## 4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

### 4.5.1 CHRONIC TOXICITY TO FISH

### 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

### 4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

### 4.6.2 TOXICITY TO TERRESTRIAL PLANTS

### 4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

### 4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

### 4.7 BIOLOGICAL EFFECTS MONITORING

### 4.8 BIOTRANSFORMATION AND KINETICS

### 4.9 ADDITIONAL REMARKS

## 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

## 5.1.1 ACUTE ORAL TOXICITY

## 5.1.2 ACUTE INHALATION TOXICITY

| | | |
|---|---|---|
| **Type** | : | other |
| **Value** | : | |
| **Species** | : | human |
| **Strain** | : | |
| **Sex** | : | |
| **Number of animals** | : | |
| **Vehicle** | : | |
| **Doses** | : | 100,000, 150,000, 200,000, 250,000, 300,000, 330,000 and 350,000 ppm |
| **Exposure time** | : | |
| **Method** | : | other |
| **Year** | : | 1925 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | It is evident from this study that the LD50 value in humans is greater than 10% (100,000 ppm). |
| **Result** | : | Inhalation of 10% caused feelings of mild intoxication with parethesia, and had a slight effect on reaction time. Fifteen percent caused distinct intoxication with talkativeness, sleepiness and inability to walk a straight line, but did not include symptoms of marked intoxication (even after an hour's inhalation). Marked intoxication was evident after inhalation of 20% for 4 minutes. Slight uncoordination of head movements was noticed after 20% had been inhaled for 18 minutes. Twenty five percent acetylene caused similar but more marked symptoms. An effect on writing, typewriting, simple reaction time or memory was not observed after inhalation of less than 20 - 25%. General uncoordination and aggressive behavior were noted after inhalation of 30% acetylene for 13 minutes. Inhalation of 33% or 35% caused unconsciousness within 7 and 5 minutes, respectively. Inhalation of 50% acetylene produced feelings of intense intoxication within 35 seconds and an unbearable feeling of suffocation in 70 seconds (after which the experiment was stopped). |
| **Test condition** | : | Humans (number and sex were not listed) were administered acetylene (10 - 50 %) from a Douglas bag in the sitting position. No re-breathing was allowed. The acetylene was obtained from the Bon-Accord Acetylene Gas Company, and was prepared from calcium carbide and purified by passing through a lime-tower. Clinical signs were monitored and the concentration that produced unconsciousness (and exposure time) was listed. The effects of acetylene inhalation on memory, reflex times and muscular movement also were assessed. |
| **Reliability** | : | (2) valid with restrictions<br>The number of humans tested was not listed. Although the purity of the material was not listed, it is assumed that it is of fairly high purity since it was purified before use. |
| **Flag** | : | Critical study for SIDS endpoint |

04.01.2007 (4)

| | | |
|---|---|---|
| **Type** | : | other |
| **Value** | : | |
| **Species** | : | rat |
| **Strain** | : | |

| | | |
|---|---|---|
| **Sex** | : | |
| **Number of animals** | : | |
| **Vehicle** | : | |
| **Doses** | : | 780,000 and 900,000 ppm |
| **Exposure time** | : | |
| **Method** | : | other |
| **Year** | : | 1925 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | This is a supporting study for the SIDS endpoint. |
| **Result** | : | A concentration of 78% acetylene (780,000 ppm) produced anesthesia in 15 minutes. Acetylene did not cause marked excitement before anesthesia.<br><br>A concentration of 90% acetylene (900,000 ppm) caused respiratory failure in approximately 2 hours. It assumed that this concentration was lethal. |
| **Test condition** | : | Acetylene and other gases were tested for inhalation toxicity in a single strain of white rats of uniform weight (number and sex of animals and details about exposure were not provided). |
| **Reliability** | : | (4) not assignable<br>Not enough details are present to assign a reliability rating. |

21.10.2003 (23)

| | | |
|---|---|---|
| **Type** | : | other |
| **Value** | : | |
| **Species** | : | dog |
| **Strain** | : | |
| **Sex** | : | |
| **Number of animals** | : | |
| **Vehicle** | : | |
| **Doses** | : | |
| **Exposure time** | : | |
| **Method** | : | other |
| **Year** | : | 1925 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Inhalation of 50 dogs to 850,000 ppm increased respiratory volume and frequency and induced anesthesia, with rapid recovery. Therefore, the LD50 value in this study is greater than 850,000 ppm. |
| **Reliability** | : | (4) not assignable<br>There are not enough data to assign a reliability rating. The original reference was not consulted. |

04.01.2007 (16)

### 5.1.3 ACUTE DERMAL TOXICITY

### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

### 5.2.1 SKIN IRRITATION

### 5.2.2 EYE IRRITATION

## 5.3 SENSITIZATION

## 5.4 REPEATED DOSE TOXICITY

| | | |
|---|---|---|
| **Type** | : | |
| **Species** | : | |
| **Sex** | : | |
| **Strain** | : | |
| **Route of admin.** | : | |
| **Exposure period** | : | |
| **Frequency of treatm.** | : | |
| **Post exposure period** | : | |
| **Doses** | : | 250,000, 500,000 and 800,000 ppm |
| **Control group** | : | |
| **NOAEL** | : | = 800000 ppm |
| **Method** | : | other |
| **Year** | : | 1933 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Remark** : This is a supporting study for the SIDS endpoint.
Since capillary hyperemia was not observed in rats exposed to higher concentrations of acetylene, it does not appear to be test-material related.

**Result** : The numbers of animals that died spontaneously are reported in the following table:

| Animal | Conc. (%) | Daily Exposure Time (hours) | Number Of Days Exposed | Total Exposure Time (hours) | Deaths |
|---|---|---|---|---|---|
| Rat | 25 | 1 | 7-93 | 7-93 | 6/16 |
| Rat | 50 | 2 | 1-8 | 2-16 | 9/10 |
| Guinea Pig | 50 | 2 | 1-9 | 2-18 | 7/7 |
| Mouse | 50 | 2 | 1-6 | 2-12 | 5/5 |
| Rat | 80 | ½ | 2-36 | 1-18 | 36/47 |
| Rat | 80 | 1 | 14 | 14 | 0/8 |
| Guinea Pig | 80 | 1 | 10 | 10 | 0/6 |
| Rabbit | 80 | 1 | 6-10 | 6-10 | 3/4 |
| Dog | 80 | 1 | 12 | 12 | 1/2 |

At the lower concentrations (concentrations were not stated) the animals appeared only slightly sleepy. At higher concentrations (70-80%), the majority of animals fell asleep after 15-20 minutes. In general, these animals were not in deep narcosis. The rats, rabbits, guinea pigs and dogs generally recovered from narcosis in a short time. However, the mice did not survive treatment. Some of the animals died spontaneously. Pneumonia was observed in most of these cases. Since pneumonia also was observed in control animals exposed only to air, it did not appear to be related to treatment. In treated animals that survived to termination, the authors found no evidence of cellular injury to the parenchymatous cells of the heart, lungs, liver, kidneys, or spleen. However, capillary hyperemia was observed in the liver, kidneys and spleen of some rats exposed to 250,000 ppm (the number was not stated). This effect was observed until at least the second day after the last exposure to the gas but was not evident in animals killed later (up to 5 days after the last exposure).

**Test condition** : Rats, mice, guinea pigs, rabbits, and dogs were exposed to acetylene in oxygen according to the scheme presented in the following table:

| Animal | No. Tested/ Deaths/ Terminated | Conc. (%) | Daily Exposure Time (hours) | Number of Days Exposed | Total Exposure Time (hours) |
|---|---|---|---|---|---|
| Rat | 16/6/12 | 25 | 1 | 7-93 | 7-93 |
| Rat | 10/9/1 | 50 | 2 | 1-8 | 2-16 |
| Guinea Pig | 7/7/0 | 50 | 2 | 1-9 | 2-18 |
| Mouse | 5/5/0 | 50 | 2 | 1-6 | 2-12 |
| Rat | 47/36/11 | 80 | ½ | 2-36 | 1-18 |
| Rat | 8/0/8 | 80 | 1 | 14 | 14 |
| Guinea Pig | 6/0/6 | 80 | 1 | 10 | 10 |
| Rabbit | 4/3/1 | 80 | 1 | 6-10 | 6-10 |
| Dog | 2/1/2 | 80 | 1 | 12 | 12 |

Thirty animals also served as controls. The number of controls for each species was not listed.

The animals were placed in glass cages that were air tight, and on one side the gassing apparatus was placed to introduce the gas, and on the other side of the cage an equal amount of air was exhausted out. This setup enabled the animals to move about freely without changes in air pressure and have the right amount of oxygen. The stream of acetylene/oxygen introduced amounted to 5 liters per minute, so that carbon dioxide buildup was ruled out for practical purposes.

As a rule, exposures were conducted daily. During the experiment, most of the animals (numbers were not stated) were weighed after various intervals. In some experiments, blood samples were taken at regular intervals from controls (numbers of animals were not stated).

Animals that survived to study termination were killed either right after the experiment or later by striking them on the head. A series of 30 controls also were killed by head strike. Three control animals showed signs of congestion from this method of killing. Most of the animals were killed and examined several hours after the last experiment. A portion was killed up to 5 or 14 days after the last exposure (individual numbers were not listed). Animals that died spontaneously the first 1-3 days after the last exposure also were examined. All animals were dissected and the organs (heart, lung, liver, kidney and spleen) were fixed in formalin or Zenker solution according to standard procedure, embedded in paraffin glycogen stain in celloiden and examined microscopically. In addition, frozen tissue slices were made and stained.

**Conclusion** : The authors concluded that acetylene did not cause any sort of histologically detectable damage to parenchymatous cells at the concentrations tested.

**Reliability** : (2) valid with restrictions
The study was not performed according to current standards.

04.01.2007 (13)

**Type** : Sub-chronic
**Species** : rat
**Sex** : male
**Strain** : other: albino
**Route of admin.** : inhalation
**Exposure period** : 6 hours per day
**Frequency of treatm.** : 5 days/week for 6 months
**Post exposure period** :
**Doses** : 28,700 ppm
**Control group** : yes, concurrent no treatment
**NOAEL** : < 28700 ppm

| | | |
|---|---|---|
| **Method** | : | other |
| **Year** | : | 1957 |
| **GLP** | : | no |
| **Test substance** | : | other TS |
| **Remark** | : | This is a supporting study for the SIDS endpoint.<br><br>An acute study performed before this study showed that inhalation of 42,000 ppm for 6 hours did not cause lethality. |
| **Result** | : | Chamber concentration: The concentration of material in the atmosphere of control animals was 2000 ppm. This was subtracted from the concentration analyzed in the atmosphere of exposed animals (30,700 ppm), to obtain a corrected exposure concentration of 28,700 ppm.<br><br>Signs of toxicity during exposure: On the first day of exposure, slight ataxia was noted within 7 minutes of exposure. After one half hour, most of the rats were lying on the chamber floor, in an early plane of anesthesia. A peculiar "pecking" motion of the head was exhibited throughout the first exposure. During remaining exposures, rats were observed to be in one position, lying either on the abdomen or on the side, with gross tremors of the head and extremities. The rats appeared to be unable to maintain balance. All animals recovered rapidly after exposures were terminated.<br><br>Signs of toxicity observed following exposure: Animals were depressed after exposure, and their fur was wet, discolored and ruffled. Rats were "unthrifty" after about 2 months on study. Eight (40%) of the rats died. Times of death were listed as 21, 34 (2 deaths), 46, 74, 95, 102 and 103 days. Two of the controls died. Over the course of the study, weight gain was slightly retarded in exposed rats.<br><br>Gross pathology of animals that died was limited to the lungs, which appeared dark red. The lungs remained distended when the thorax was opened, but no edema fluid was found. On palpation, the lungs had a firm consistency. A purulent empyema was observed in one rat.<br><br>In exposed rats that survived to termination, the lungs also were discolored and remained distended. Discoloration ranged from speckled red areas to a homogeneous, dark red, hemorrhagic appearance. Cut sections of lungs were a homogeneous, dark red color and either edema fluid or blood could be expressed from them. Lungs from 3 of the 12 surviving animals had cysts which contained a "cheesy material". The remaining organs appeared to be within normal limits. Microscopic pathology of the lungs showed definite pulmonary irritation. |
| **Test condition** | : | Animals: A group of 20 male albino rats (avg. weight 135 g) were exposed to an average concentration of 28,700 ppm methylacetylene for 6 hours/day, 5 days/week for 6 months. An equal number of rats was housed in the same laboratory to serve as controls. The laboratory temperature was 25 +/- 1 degrees C.<br><br>Exposure: Exposures were performed in 500 liter, stainless steel chambers with a water-sealed lid. The inlet was equipped with a suitable device to inject methylacetylene vapor, and the outlet was equipped with an orifice flowmeter, control valve and exhaust pump. Methylacetylene vapor was injected into the inlet at a fixed rate of flow from a large steel cylinder. A constant rate of flow was maintained during exposure with a reducing pressure valve and an orifice flowmeter, which was connected to a water manometer. The flow was constantly monitored. Methylacetylene was mixed with room air, which was drawn into the exposure chamber.<br><br>Test conduct: Animals were observed for signs of toxicity during and after exposure (specific times were not listed). Animals were observed at least daily for mortality. Animals were weighed on days 0, 13, 24, 31, 38, 45, 60, |

64, 71, 76, 85, 95, 102, 109, 120, 127, 137, 141, 146, 158, 165, 173, 179 and at termination (date was not stated). Gross pathologies of animals that died were performed as soon as possible after death. Gross pathologies of animals that survived the course of treatment were performed upon termination. Sections of lung, liver, kidney, heart, spleen and GI tract were examined microscopically.

Concentration of Test material: The concentration of material in the chamber was determined by drawing a known volume of the chamber atmosphere (measured with a wet-test meter) through 6 bubblers (in series) containing methanol. Samples were not drawn until the chamber concentration had equilibrated. The concentration of test material in each bubbler was determined separately. If an appreciable mount of material was found in the last bubbler, the samples were drawn at a slower rate. Blank samples from chambers containing control animals were run to determine the contribution of animal metabolites.

Solution from each bubbler was placed into a 250 ml volumetric flask, containing 50 ml of potassium mercuric iodide and 50 ml of 0.5 N sodium hydroxide. Methanol was added to make the contents up to 250 ml. The mixture was shaken and a 25 ml aliquot was titrated with 0.5 N sulfuric acid, using phenolphthalein as an indicator.

**Test substance** : The test material was methylacetylene (also known as propyne). Purity of the material is unknown.

**Reliability** : (2) valid with restrictions
Only one concentration was tested. The study is not as rigorous as a guideline study.

04.01.2007 (17)

| | | |
|---|---|---|
| **Type** | : | Sub-chronic |
| **Species** | : | dog |
| **Sex** | : | male/female |
| **Strain** | : | |
| **Route of admin.** | : | inhalation |
| **Exposure period** | : | 6 hours per day |
| **Frequency of treatm.** | : | 5 days/week for 6 months |
| **Post exposure period** | : | |
| **Doses** | : | 28,700 ppm |
| **Control group** | : | yes, concurrent no treatment |
| **NOAEL** | : | < 28700 ppm |
| **Method** | : | other |
| **Year** | : | 1957 |
| **GLP** | : | no |
| **Test substance** | : | other TS |

**Remark** : This is a supporting study for the SIDS endpoint.

**Result** : Chamber concentration: The concentration of material in the atmosphere of control animals was 2000 ppm. This was subtracted from the concentration analyzed in the atmosphere of exposed animals (30,700 ppm), to obtain a corrected exposure concentration of 28,700 ppm.

Signs of toxicity during exposure: On the first day of exposure, marked salivation, excitability and muscular fasciculations were noted within 7 minutes of exposure. After 13 minutes, the dogs exhibited ataxia and mydriasis. After 30 minutes, one dog was lying on the chamber floor, in an early plane of anesthesia. One dog did not eat following the first exposure. Throughout the remaining exposures, similar signs of toxicity were observed. In addition, within 15 minutes of exposure, dogs appeared to be intoxicated (similar to alcohol). The dogs were excited and walked about the chamber, occasionally staggering and falling on the floor or against the sides. Shortly after termination of exposure, the dogs would lie quietly on the chamber floor.

Tonic convulsions occurred in at least one of the dogs on days 22, 110, 123 and 137. There was a prodromal syndrome consisting of 15-30 minutes of hyperexcitability, which terminated in a tonic convulsion of a few minutes' duration. Dogs recovered soon after the episodes.

Exposed dogs lost weight during the first 6 weeks of the experiment, attained their initial weight by week 14, and continued to gain weight until termination.

There was no effect of treatment on any hematological, urine or biochemical index of toxicity. The gross appearance of all organs (specific organs examined were not listed) and microscopic examinations of the lung, liver, kidney, heart, spleen and GI tract in exposed animals were normal.

**Test condition** **:** Animals: Two dogs (one male and one female) weighing 7.6 and 9.0 kg, respectively, were exposed to an average concentration of 28,700 ppm methylacetylene for 6 hours/day, 5 days/week for 6 months. Two male dogs were housed in the same laboratory to serve as controls. The laboratory temperature was 25 +/- 1 degrees C.

Exposure: Exposures were performed in 500 liter, stainless steel chambers with a water-sealed lid. The inlet was equipped with a suitable device to inject methylacetylene vapor, and the outlet was equipped with an orifice flowmeter, control valve and exhaust pump. Methylacetylene vapor was injected into the inlet at a fixed rate of flow from a large steel cylinder. A constant rate of flow was maintained during exposure with a reducing pressure valve and an orifice flowmeter which was connected to a water manometer. The flow was constantly monitored. Methylacetylene was mixed with room air, which was drawn into the exposure chamber.

Test conduct: Animals were observed for signs of toxicity during and after exposure (specific times were not listed). Animals were observed at least daily for mortality. Animals were weighed on days 0, 13, 24, 31, 38, 45, 60, 64, 71, 76, 85, 95, 102, 109, 120, 127, 137, 141, 146, 158, 165, 173, 179 and at termination (date was not stated).

Blood samples were taken for analysis of sedimentation rate, hematocrit, hemoglobin and white blood cell count at approximately 10-day intervals. Biochemistries consisting of icterus index, blood urea nitrogen, blood sugar, plasma chloride, and plasma carbon dioxide combining power and urinalyses (appearance, reaction, specific gravity, protein, sugar, occult blood and microscopic examination) were also performed at approximately 10-day intervals. Sulfobromophthalein sodium (BSP) tests were done at various intervals by administering a dose of 5.0 mg/kg to each dog and drawing blood samples 15 and 30 minutes later. The percent retention of BSP was determined by comparing the values to those of standards. Blood volumes were determined by injecting 1 ml of Evans blue dye and drawing blood 10 minutes later.

Gross pathologies of animals that died were performed as soon as possible after death. Gross pathologies of animals that survived the course of treatment were performed upon termination. Sections of lung, liver, kidney, heart, spleen and GI tract were examined microscopically.

Concentration of Test Material: The concentration of material in the chamber was determined by drawing a known volume of the chamber atmosphere (measured with a wet-test meter) through 6 bubblers (in series) containing methanol. Samples were not drawn until the chamber concentration had equilibrated. The concentration of test material in each bubbler was determined separately. If an appreciable amount of material was found in the last bubbler, the samples were drawn at a slower rate.

Blank samples from chambers containing control animals were run to determine the contribution of animal metabolites.

Solution from each bubbler was placed into a 250 ml volumetric flask, containing 50 ml of potassium mercuric iodide and 50 ml of 0.5 N sodium hydroxide. Methanol was added to make the contents up to 250 ml. The mixture was shaken and a 25 ml aliquot was titrated with 0.5 N sulfuric acid, using phenolphthalein as an indicator.

**Test substance** : The test material was methylacetylene (also known as propyne). Purity of the material is unknown.

**Reliability** : (2) valid with restrictions
Only one concentration was tested in 2 dogs. The study is not as rigorous as a guideline study.

04.01.2007 (17)

## 5.5 GENETIC TOXICITY 'IN VITRO'

**Type** : Ames test
**System of testing** : Salmonella typhimurium TA97, TA98, TA100
**Test concentration** : up to 31 micrograms/plate
**Cytotoxic concentr.** :
**Metabolic activation** : with and without
**Result** : negative
**Method** : other
**Year** : 1984
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Remark** : The test conditions used in the study were previously determined in a preliminary study that examined the 1) toxicity and mutagenicity of styrene oxide with log- and stationary-phase cells of TA100 with pre-incubation or plate incorporation, 2) mutagenicity testing of methylene chloride with the plate incorporation and preincubation techniques, 3) the effect of head-space volume and different types of shaking (during preincubation) on the mutagenic potential of styrene oxide and methylene chloride, 4) the effect of solvents and metabolic activation on the mutagenic potential of vapor-phase mutagens, and 5) the effect of preincubation time (10 - 60 min) on the mutagenic potential of styrene oxide. The results indicated that the optimal system used preincubation (10-30 minutes) with log-phase cells in full vials that were not shaken during preincubation.

The concentrations used were lower than that recommended in guideline tests (5000 micrograms/plate) due to limited solubility in the solvent.

**Result** : There was no effect of acetylene on the number of mutants in the absence of S-9. The average number of mutants in control strains TA97, TA98 and TA100 without S-9 were 142, 25.7 and 184.7, respectively. The average number of mutants in treated strains TA97, TA98 and TA100 without S-9 ranged from 97- 106.3, 17.3 - 27.7 and 145.3 - 227.0, respectively.

There was no effect of acetylene on the number of mutants in the presence of rat S-9. The average numbers of mutants in control strains TA97, TA98 and TA100 with rat S-9 were 167.3, 34.3 and 174.0, respectively. The average number of mutants in treated strains TA97, TA98 and TA100 with rat S-9 ranged from 131.3- 144.7, 23.3 - 34.7 and 119.0 - 157.7, respectively.

There was no effect of acetylene on the number of mutants in the presence of hamster S-9. The average numbers of mutants in control strains TA97, TA98 and TA100 with hamster S-9 were 184.0, 38.3 and 199.7, respectively. The average number of mutants in treated strains TA97,

TA98 and TA100 with hamster S-9 ranged from 121.7- 149.7, 23.3 - 36.0 and 144.7 - 167.7, respectively.

The test was valid, since both concentrations of each positive control induced at least a two-fold increase in the number of mutants with respect to solvent controls.

**Test condition** : Salmonella typhimurium strains TA97, TA98 and TA100 were obtained from Dr. Bruce Ames, University of California, Berkeley. Stationary cells were grown overnight (16 hours) with shaking at 50 rpm; log-phase cells were grown on the day of the experiment by inoculating a fresh nutrient broth culture with fresh overnight culture (1:10 dilution) and shaking the culture for 4 hours at 50 rpm and 37 +/- 0.5 degrees C. Plates were incubated for 48 hours, and colonies were counted with a calibrated automatic cell counter.

Rat and hamster liver S9 were derived from male Sprague-Dawley rats and male Syrian Golden hamster, respectively. Both rats and hamsters were induced with 500 mg/kg Aroclor 1254 five days before liver harvest.

Positive controls were as follows: 50 and 100 micrograms/plate 9-aminoacridine for TA97 without S-9, 1 and 2 micrograms/plate 2-nitrofluorene for TA98 without S-9, 1 and 2 micrograms/plate sodium azide for TA100 without S-9, 1 and 2 micrograms/plate 2-aminoanthracene for all strains with rat S-9, and 0.5 and 1 micrograms/plate for all strains with hamster S-9.

Test vials contained (per plate): 500 microliters of medium or 5% S9 mix, 100 microliters of bacteria (cell number was not indicated), 100 microliters of acetylene (0.3, 1, 3, 10, or 31 micrograms/plate) in acetone solvent, acetone alone (negative control) or positive control, and 600 microliters of overlay agar. Test concentrations were chosen based on the results of a preliminary toxicity and solubility studies. Each vial contained the contents for 3 plates (without headspace). Vials were preincubated for 10 min at 37 degrees C in sealed one-dram glass vials in a temperature-controlled exposure chamber that completely surrounded the glass vial. The vial was not shaken during preincubation. Toxicity was determined by plating approximately 1,000 colonies on histidine-supplemented agar. A viability index was calculated by comparing the number of colonies present on a dosed plate to a solvent control plate. A viability index below 50% indicated excessive toxicity. A positive response was defined as at least a two-fold increase in the number of mutants in treated cells vs. solvent controls at two increasing dose levels.

Aliquots of each sample used in the Ames test were removed (times were not stated) and assayed for acetylene concentration by GC analysis [6' chromosorb 102 packed 1/4" glass GC column (at 100 degrees C) with FI detection]. Each sample was assayed in triplicate, and mean concentration was calculated from the standard curve. Standards of test material were prepared by filling an evacuated 0.5 l gas bulb with acetylene and allowing the pressure to equilibrate to 1 atm. Samples were withdrawn through a septum in the bulb with a gas-tight syringe and chromatographed as described above. Duplicate injections were made for each point and a response curve of a least 3 points was established.

**Test substance** : Purity of the test material was not given; however it was mentioned that the material was obtained from Matheson Gas Company and was of the highest quality available.

**Reliability** : (2) valid with restrictions
Only three strains were used in the study.

**Flag** : Critical study for SIDS endpoint
04.01.2007 (18)

**Type** : Bacterial reverse mutation assay

| | | |
|---|---|---|
| **System of testing** | : | S. typhimurium TA98, TA100, TA1535 and TA1537 and E. coli WP2uvrA |
| **Test concentration** | : | 0, 5, 10, 21 and 50% |
| **Cytotoxic concentr.** | : | no data |
| **Metabolic activation** | : | with and without |
| **Result** | : | |
| **Method** | : | other |
| **Year** | : | 1994 |
| **GLP** | : | no data |
| **Test substance** | : | other TS |

**Remark** : Fifteen different gases were tested in the study. Some of the materials caused dose-dependent increases in revertants in the absence and presence of S9, and others did not. Results obtained in the study were similar to those reported by others, which validated the model. It is unknown why the results at 5 and 10 % in the absence of S9 were not considered to be positive, since the number of mutants appears to be at least twice that of the control. However, it is difficult to determine the exact number since the results were depicted graphically, with tic marks on the x axis (number of revertants) placed at 50.

It is unknown whether the concentrations tested were cytotoxic.

**Result** : Methyl acetylene did not cause an increase in mutations in any strain of Salmonella at any concentration in the absence or presence of S9 mix. Methylacetylene caused a dose dependent increase in the number of mutations in E. coli WP2 uvra in the absence or presence of S9 mix. The authors stated that the effect was positive at concentrations > = 21% without S9 mix (approximately > = 100 revertants/plate were detected) and > = 5% with S9 mix (approximately > = 75 revertants/plate were detected). The number of revertants in the controls with and without S9 mix was < 25/plate.

**Test condition** : Bacteria: S. typhimurium TA98, TA100, TA1535 and TA1537 were supplied by Dr. Bruce Ames, University of California, Berkeley and E. coli WP2 uvrA was supplied by Dr. M Ishizawa, Kyushu University, Fukuoka Japan. Stock cultures were stored at -80 degrees C. Bacteria were subcultured for 10 hours in nutrient broth before use.

S9 and S9 mix: Liver homogenate (S9) was prepared from male Sprague Dawley rats (6 weeks old). Phenobarbital and 5,6-benzoflavone were used as inducers. The S9 mix contained 4 mM NADPH, 4 mM NADH, 5 mM glucose 6-phosphate, 8 mM MgCl2, 33 mM KCl, 100 mM sodium phosphate buffer (pH 7.4) and 10-40% S9.

Exposure system: Gas from the cylinder was collected into a 20-liter gas sampling bag. Another 20-liter gas sampling bag was filled with dilution gas (HEPA-filtered air). A fixed volume of the test gas was pumped out from the gas sampling bag and pumped into another gas sampling bag (gas dilution bag), which had been filled with a fixed amount of the dilution gas using a flowmeter and pump. The gas dilution bag was squeezed by hand to mix the gases. The concentrations used in the test were calculated using the volumes of test and dilution gases.

Test material concentration: The concentration of gas in the bag was measured at the beginning of exposure using gas chromatography with FID/TCD detection. One ml of sample was withdrawn through the septum of the bag using a gas-tight syringe. Separations were performed using a Polapak Q column (3 mm x 2 m) or Silicone DC 550 column (3 mm x 2 m). Column temperature, injection temperature, and gas flow (N or He) were 70 degrees C, 120 degrees C and 50 ml/min, respectively. Concentrations used in the test were 0 (control), 5, 10, 21 and 50%.

Mutation test: Bacterial plates were prepared using the spread method and the agar overlay method. For the spread method, 0.2 ml of a 0.5 mM

histidine/biotin (for S. typhimurium) or 0.2 ml of a 0.5 mM L-tryptophan (for E coli) solutions were poured into sterile tubes, to which 0.5 ml of a 0.1 M phosphate buffer or S9 mix was added. Test bacteria (0.1 ml) were added and the entire solution was spread onto a minimal glucose agar plate. For the agar overlay method, 0.5 ml of a 0.1 M phosphate buffer or S9 mix was mixed with 0.1 ml of bacteria. Immediately after adding 1 or 2 ml of top agar containing 0.1 micromoles of L-histidine/D-biotin or L-tryptophan, the mixture was poured onto minimal glucose agar plates. Based on the results of a preliminary study with 1,3-butadiene (see below), it is assumed that the agar overlay method was used to test methyl acetylene.

Prepared plates were placed upside down (without lids) in a plate holder and the plate holder was placed in a 10-liter gas sampling bag through a hole cut with scissors. The hole was sealed by folding the opening 2 or 3 times and securing the fold with adhesive tape. The air in the bag was removed with a pump to check that the bag was air-tight. A flow meter and pump were connected to the gas dilution bag and approximately 1 liter of the test gas (at a known concentration) was pumped into the gas exposure bag. The gas in the exposure bag was then sucked out with a pump and the remaining air in the exposure bag was washed out. After washing out the air, the gas exposure bag was filled with the test gas at a fixed amount per plate. The plates were kept at 25 or 37 degrees C (exact temperature was not listed) for a "fixed period". It is assumed that exposure time was 14 hours based on the preliminary study with 1,3-butadiene (see below). After exposure was terminated, the gas in the exposure bag was removed, HEPA-filtered air was pumped into the exposure bag and the plates were removed. The plates were placed in a hood for 30 minutes to allow the test material to evaporate and lids were placed on them. The plates were then incubated inverted for 24 hours at 37 degrees C.

The conditions listed above were chosen based on the results of a preliminary study with 1,3 butadiene, in which the effect of the volume of gas per plate (357, 625, 1250, 2500 or 5000 ml/plate, which corresponded to 14, 8, 4, 2 or 1 plates/bag), the amount of S9 (50, 100, 200 or 400 microliters/plate), the exposure temperature (30 or 37 degrees C), exposure period (2, 4, 14, 24 or 48 hours), and amount of top agar (0, 1, or 2 ml/plate) were examined. For each experiment, one factor was changed at a time. 1,3 butadiene was not mutagenic if the exposure period was < 4 hours and was optimally mutagenic after 14 hours of exposure. The rate of mutagenicity was lower if bags contained 1-4 plates. A concentration of 100 microliters/ plate S9 was optimal. Exposure temperature did not have a significant effect. The agar overlay method was more sensitive than the spread method. The conditions used for the gases optimized the chances for a positive result while conserving resources.

**Test substance** : The test material was propyne (CAS No. 74-99-7, methyl acetylene), used as supplied by Tokyo Kasei Co. Ltd.

**Reliability** : (2) valid with restrictions
Criteria for a positive or negative test were not given. Cytotoxicity was not determined. Purity of the test material is unknown.

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**Type** : Chromosomal aberration test
**System of testing** : Chinese Hamster Lung (CHL)
**Test concentration** : Experiment 1:
6(18)-h (+/-S9): 0, 0.16, 0.32, 0.625, 1.25 (% in air)
Experiment 2:
24-h (-S9): 0, 0.04, 0.08, 0.156, 0.313, 0.625, 1.25 (% in air)
6(18)-h (+S9): 0, 0.04, 0.08, 0.156, 0.313, 0.625, 1.25 (% in air)
**Cytotoxic concentr.** : >1.25% in air
**Metabolic activation** : with and without
**Result** : negative
**Method** : OECD Guide-line 473

| | | |
|---|---|---|
| **Year** | : | 2006 |
| **GLP** | : | yes |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | The upper dose level investigated, 1.25% in air, was set by the Sponsor as half the Lower Explosive Level (LEL) of acetylene (2.5% in air, National Fire Protection Association, 1997). |
| **Result** | : | Preliminary Toxicity Test:<br>The dose range used in the preliminary toxicity test was 0.02 to 1.25% in air. Microscopic assessment of the slides prepared from the exposed cultures showed that metaphase cells were present at dose levels up to 1.25% in air in the 6(18)-hour with and without-S9 exposure groups and the 24-hour continuous exposure group without-S9. In all cases the test material showed no evidence of cell toxicity (cell counts at the highest concentration +/-S9 ranged from 79 - 138% of control values).<br><br>The dose selection for the main experiments was based on the maximum proposed dose level of 1.25% in air.<br><br>Chromosome Aberration Test - Experiment 1: The maximum dose selected for metaphase analysis was 1.25% in air, the maximum dose level designated in the protocol.<br><br>Both of the vehicle control groups had frequencies of cells with chromosome aberrations within the expected range. The positive control materials induced statistically significant increases in the frequency of cells with aberrations. The metabolic activation system was therefore shown to be functional and the test method itself was operating as expected.<br><br>The test material induced a small but statistically significant increase in the frequency of cells with aberrations at 0.32% in the presence of metabolic activation (S9). The increase was very modest, only marginally exceeded the historical range for this dose group, was not part of a dose-related response and was not repeated in Experiment 2; therefore, it was considered to be artefactual and of no toxicological significance. No increases in the frequency of cells with aberrations were observed in the absence of S9. The test material did not induce any statistically significant increases in the number of polyploid cells at any dose level in either exposure group.<br><br>Chromosome Aberration Test - Experiment 2:<br>The test material induced expected levels of toxicity similar to that observed in the preliminary Toxicity Test. Therefore the maximum dose selected for metaphase analysis was 1.25% in air, the maximum dose level designated in the protocol.<br><br>Both of the vehicle control groups had frequencies of cells with chromosome aberrations within the expected range. The positive control materials induced statistically significant increases in the frequency of cells with aberrations. The metabolic activation system was therefore shown to be functional and the test method itself was operating as expected.<br><br>The test material induced a small but statistically significant increase in the frequency of cells with aberrations in the 24-hour continuous exposure group. The increase seen at 0.625% was very modest and within the historical range for the vehicle control for this dose group and with no evidence of a response in Experiment 1 was, therefore, considered to be of no toxicological significance. No increases in the frequency of cells with aberrations were observed in the 6(18)-hour pulse exposure group with a 2% final S9 concentration. This was taken to confirm that the modest response observed in Experiment 1 was of no biological relevance. The test material did not induce any statistically significant increases in the |

numbers of polyploid cells at any dose level in either exposure group.

**Source** : Safepharm Laboratories Derby

**Test condition** : METABOLIC ACTIVATION: S9 from rat liver, induced with phenobarbitone and B-naphthoflavone

POSITIVE CONTROLS:

-S9 mix: Mitomycin C (MMC) dosed at 0.1 µg/mL in Experiment 1 and 0.0.5 µg/mL for Experiment 2.
+S9 mix: Cyclophosphamide (CP) dosed at 7.5 µg/mL in Experiment 1 and 5.0 µg/mL in Experiment 2.

Experiment 1:
Short term test (+/- S9 mix): 6 hours exposure to the test material (+/- S9 mix) followed by 18 hours culture in treatment-free medium prior to cell harvest [referred to as 6(18)-h (+/-S9) above].

Experiment 2:
Short term test (+S9 mix): 6 hours exposure to the test material (+S9 mix) followed by 18 hours culture in treatment-free medium prior to cell harvest [referred to as 6(18)-h (+S9) above].

Continuous exposure without activation: 24 hours continuous exposure to the test material without S9 mix prior to cell harvest [referred to as 24-h (-S9) above].

**Conclusion** : The test material did not induce any toxicologically significant or dose-related increases in the frequency of cells with structural or numerical chromosome aberrations either in the presence or absence of a liver enzyme metabolizing system or after various exposure times. The test material was therefore considered to be non-clastogenic to CHL cells in vitro.

**Reliability** : (1) valid without restriction
Guideline study conducted under GLP

**Flag** : Critical study for SIDS endpoint

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## 5.6 GENETIC TOXICITY 'IN VIVO'

## 5.7 CARCINOGENICITY

## 5.8.1 TOXICITY TO FERTILITY

## 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

## 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

## 5.9 SPECIFIC INVESTIGATIONS

## 5.10 EXPOSURE EXPERIENCE

### 5.11 ADDITIONAL REMARKS

## 6.1 ANALYTICAL METHODS

## 6.2 DETECTION AND IDENTIFICATION

## 7.1 FUNCTION

## 7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

## 7.3 ORGANISMS TO BE PROTECTED

## 7.4 USER

## 7.5 RESISTANCE

## 8.1 METHODS HANDLING AND STORING

## 8.2 FIRE GUIDANCE

## 8.3 EMERGENCY MEASURES

## 8.4 POSSIB. OF RENDERING SUBST. HARMLESS

## 8.5 WASTE MANAGEMENT

## 8.6 SIDE-EFFECTS DETECTION

## 8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

## 8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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## 10.1 END POINT SUMMARY

## 10.2 HAZARD SUMMARY

## 10.3 RISK ASSESSMENT